ESA Climate Change Initiative (CCI)

Product User Guide (PUG) for the XCO_2 SCIAMACHY Data Product BESD

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

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1 Summary

This document is the Product User Guide (PUG), which is a deliverable of the ESA project GHG-CCI. The GHG-CCI project started on 1st September 2010. The GHG-CCI project is one of several projects of ESA's Climate Change Initiative (CCI). The GHG-CCI project will deliver the Essential Climate Variable (ECV) Greenhouse Gases (GHG). State-of-the-art retrieval algorithms for remote sensing of the ECV "Greenhouse Gases" (GHGs) will be developed further in the frame of this project. Multi-year Carbon Dioxide (CO2) and Methane (CH4) data sets will be generated and validated.

Two existing satellite sensors will be used to produce the core GHG-ECV products (XCO2 and XCH4): SCIAMACHY on ENVISAT and TANSO on GOSAT. Both instruments measure NIR/SWIR spectra of reflected solar radiation and are sensitive to CO2 and CH4 concentration changes close to the Earth's surface. Consequently they carry information on regional surface fluxes. The accuracy requirements for such an application are demanding, especially for CO2 but also for CH4. A two-year, round-robin exercise has been conducted for eight different CO2 and CH4 retrieval algorithms, as developed for SCIAMACHY and GOSAT. During the round-robin phase of the projects the performance of algorithms has been compared and validated with independent ground based measurements and algorithms have been select to provide input to the Climate Research Data Package (CRDP). For some products it was not possible to select one algorithm because different algorithms compared equally well with the validation measurements but showed significant differences at a global scale. An overview of the selected algorithms is provided in Table 1.

This document describes the BESD XCO2 data products so that it will be clear for the user how to use the products. The description includes quality flags and metadata, data format, product grid and geographical projection, known limitations, available tools for decoding and interpreting the data, and the product (column) averaging kernels and a description how to use them.

Product	Competing Algorithms	Selected Algorithms
XCO_2 SCIA	WFMD (Weighting Function Modified DOAS, IUP-Bremen) BESD (BESD Bremen optimal EStimation Doas, IUP-Bremen)	BESD
XCO_2 GOSAT	OCFP (OCO Full Physics, UoL) SRFP (SRON Full Physics, SRON)*	OCFP & SRFP
XCO_2 merged („EMMA“)	N/A	Ensemble algorithm/product -> Add to GHG-CCI portfolio

XCH_4 SCIA	WFMD IMAP (Iterative Maximum A Posteriori method, SRON / JPL)	WFMD & IMAP
XCH_4 GOSAT	OCFP +OCPR (OCO-Proxy, UoL) SRFP + SRPR (SRON-Proxy, SRON)	SRFP & OCPR

Table 1: Algorithms evaluated and selected during the round-robin phase of the GH- CCI project. * The SRFP algorithms is commonly known as RemoteC and is being jointly developed by SRON and KIT.

2 Introduction

2.1 The SCIAMACHY Instrument

The SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY, **/Burrows et al., 1995/**, **/Bovensmann et al., 1999/**) instrument started its operation in 2002 with the launch of the ESA (European Space Agency) satellite ENVISAT (Environmental Satellite) on March 1st, 2002. Roughly one decade later on May 9th, 2012 ESA declared end of the mission due to the unexpected loss of ENVISAT.

SCIAMACHY was the first and during seven years the only satellite instruments which was able to measure the CO_2 mixing ratio (XCO_2) with large sensitivity also in the boundary layer where the signals from the sources and sinks at the surface are largest.

ENVISAT was in a sun synchronous descending orbit with an equator crossing time of 10:00. SCIAMACHY measured simultaneously the radiance in 8 spectral channels in the range from 240-2400nm each consisting of 1024 spectral points. BESD uses SCIAMCHY measurements within two spectral bands, namely the O_2-A absorption band at around 760nm and the weak CO_2 absorption band at around 1580nm. The spectral resolution of these bands was 0.42nm and 1.45nm, respectively. The measurements in these bands had a ground pixel size of approximately 60km across track and 30km along track. The swath width of SCIAMACHY was about 960km.

2.2 The BESD XCO_2 Full Physics Product

The Bremen Optimal Estimation DOAS (BESD) algorithm is designed to analyze SCIAMACHY sun normalized radiance measurements to retrieve the column-average dry-air mole fraction of atmospheric CO_2, i.e., XCO_2. BESD is a so called full physics algorithm which uses measurements in the O_2-A absorption band to retrieve scattering information of clouds and aerosols. This information is transferred to the CO_2 absorption band at 1580 nm by simultaneously fitting the spectra measured in both spectral regions. The explicit consideration of scattering by this approach reduces potential systematic biases due to clouds or aerosols. More details on BESD can be found in the publications of **/Reuter et al., 2010/** and **/Reuter et al., 2011/**. As an example, Figure 2-1 shows a global map of the long term seasonal averages April/May/June (top) short before the growing season with largest values on the northern hemisphere and July/August/September (bottom) during the growing season with lowest values on the southern hemisphere.

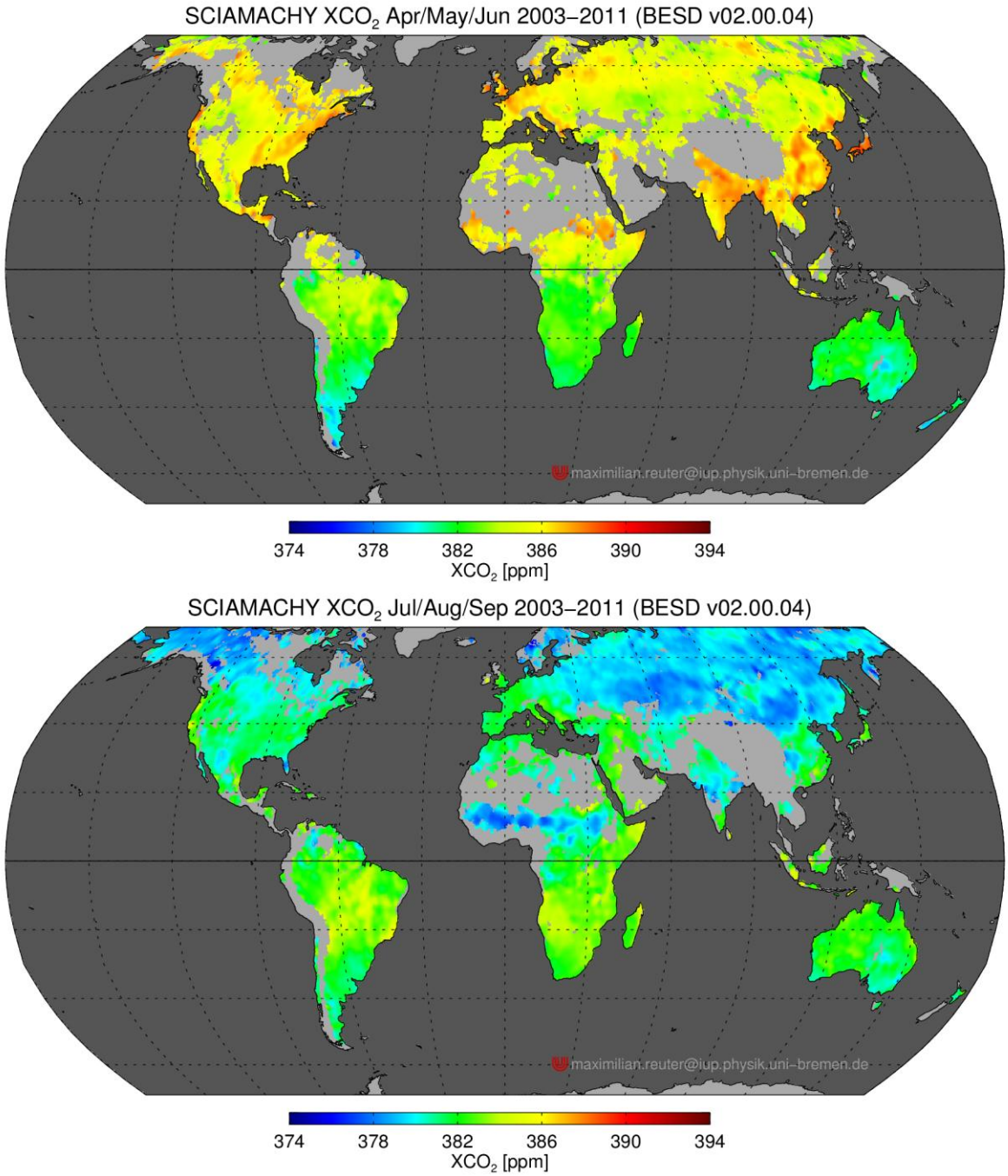

Figure 2-1: Long term seasonal averages of XCO2 retrieved with BESD. Top: April/May/June. Bottom: July/August/September.

3 Product Description

3.1 Product Content and Format

BESD results are stored in one NetCDF file per day. The file names follow the convention CO2_SCI_BESD_vXX.XX.XX_YYYYMMDD.nc where XX.XX.XX stand for a version number and YYYYMMDD stand for year month and day. The files include individual level 2 retrieval results. No averaging has been applied so that each entry corresponds to an individual SCIAMACHY spatial footprint. A table with the full content of the data product is provided in Section 3.7. The product file contains the key product, i.e. the retrieved column averaged dry air mixing ratio XCO_2 and information relevant for the use of the data like geo-location, time, vertical layering, averaging kernels, and error estimates.

3.2 Quality Flags and Metadata

BESD data are already quality filtered and include only pixels assumed to be reliable so that an additional data filtering by the user is not required. The performed quality filtering relies not on assumptions about realistic XCO_2 values. Only XCO_2-independent retrieval outputs such as fit residuals, scattering parameters, albedo or instrument related information such as the time of decontamination phases has been used.

3.3 Bias Correction

Bias correction is an integral part or the BESD retrieval algorithm, i.e., all XCO_2 values within the data files are already bias corrected. BESD's bias correction relies on a multi-dimensional non-linear regression realized by an artificial neural network (ANN). In order to give an impression of the magnitude of the bias correction: the bias correction reduces the standard error relative to TCCON validation data from about 2.7ppm to 2.1ppm.

3.4 Data Usage

It is recommended to use BESD data as provided within the data files.

If the data is to be used within in a surface flux inversion framework or if the data is compared with other XCO_2 data for which vertical profile information is available, the column averaging kernels should be used. It should be noted that the values within BESD's CO_2 and averaging kernel profiles correspond to layer averages whereas the layering is defined by the pressure profile giving the level boundaries starting with the surface pressure. This means one could expect to find pressure profiles having one element more than the CO_2 profiles. However, this is not the case because the upper most pressure level at the top of the atmosphere is always 0hPa and was omitted, therefore.

For all retrieval comparisons, it is recommended to define a common a priori ($CO_2^{common\ a\ priori}$) which is used to adjust the retrieved CO_2 ($CO_2^{retrieved}$) using the averaging kernel (A) and the original a priori ($CO_2^{original\ a\ priori}$):

$$CO_2^{adjusted} = CO_2^{retrieved} + (1 - A) \cdot \left(CO_2^{common\ a\ priori} - CO_2^{original\ a\ priori}\right)$$

As BESD's pressure levels are equally spaced, column averages (XCO_2) can then be calculated by simply averaging over the layers of the adjusted profiles.

3.5 Tools for Reading the Data

The data are stored in Netcdf format which can be read with standard tools in the common programming languages (IDL, Matlab, Python, Fortran90, C++, etc).

HDFView (http://www.hdfgroup.org/hdf-java-html/hdfview/) is a great platform independent tool with graphical user interface which can be used to have a first look what is in the data files.

3.6 Known Limitations and Issues

- Due to instrument issues data earlier than April 2003 are less reliable.

3.7 Data file content

Table 3-1: Full Data content of the CO2_SCI_BESD data products (n=number of observations, m=number of pressure levels).

Name	Type	Dimensions	Units	Description
instrument	String	1		SCIAMACHY
l2_processing_institute	String	1		IUP
l2_processor_version	String	1		Processor Version Number
l1b_input_filename	String	1		L1B Filename
solar_zenith_angle	Float	n	Degrees	Solar Zenith Angle (0°=zenith)
viewing_zenith_angle	Float	n	Degrees	Viewing Zenith Angle(0°=nadir)
azimuth_difference	Float	n	Degrees	Azimuth Difference
time	Double	n	Seconds	Seconds since 01.01.1970 00:00 UTC
longitude_centre	Float	n	Degrees	Longitude of pixel centre
latitude_centre	Float	n	Degrees	Latitude of pixel centre
longitude_corners	Float	n x 4	Degrees	Longitude of pixel corners
latitude_corners	Float	n x 4	Degrees	Latitude of pixel corners
surface_elevation	Float	n	km	Mean surface elevation of pixel
pressure_levels	Float	n x m	hPa	Retrieval pressure levels
column_averaging_kernel	Float	n x m		Normalised Column Averaging Kernel Profile

chi2	Float	n		Chi-Square of fit residual
rms	Float	n x 3		RMS of fit residual (total, O_2, CO_2)
xco2	Float	n	ppm	Retrieved XCO_2
xco2_uncertainty	Float	n	ppm	Uncertainty in retrieved XCO_2
xco2_apriori	Float	n	ppm	A priori XCO_2
vmr_profile_co2	Float	n x m	ppm	Retrieved CO_2 profile
vmr_profile_co2_uncertainty	Float	n x m	ppm	Uncertainty in retrieved CO_2 profile
vmr_profile_co2_apriori	Float	n x m	ppm	A priori CO_2 profile

4 References and Further Reading

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